Appl. No. 10/643,545
Amdt. Dated Feb. 17, 2005
Reply to Office Action of September 22, 2004

PATENT
Atty. Dkt. No. 83394.0012
Customer No. 26021

Amendments to the Claims:

This listing of claims will replace all prior versions, and listings, of claims in the application:

Listing of Claims:

1. (Original) An apparatus for analyzing mass spectrometric data comprising:

a first input means for entering first data of an ion to be analyzed measured by mass spectrometry;

a second input means for entering second data of a dissociated ion of the ion measured by mass spectrometry;

a first data storing means for storing third data of mass spectrometry of a plurality of candidates for the structure of ion;

a calculation means for producing fourth data of mass spectrometry of dissociated ions to be used in analyzing the plurality of candidates; and

an evaluation means for evaluating the plurality of candidates by making comparisons between the first and third data and between the second and fourth data, so that the structure of ion can be identified.

2. (Original) An apparatus according to claim 1, wherein the first, second, third and fourth data include mass-to-charge ratios and ion intensities, respectively.

3. (Original) An apparatus according to claim 1, wherein the calculation means executes a molecular orbital calculation for each candidate so that the fourth data can be obtained by calculation.

4. (Original) An apparatus according to claim 1, wherein the evaluation means comprises a selection means for selecting a candidate for the structure of ion

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by comparing the first and third data, the calculation means is able to calculate mass spectrometric data for a dissociated ion of the candidate selected by the selection means and the evaluation means evaluates the candidate by comparing the first data and the mass spectrometric data calculated for the candidate by the calculation means.

5. (Original) An apparatus according to claim 1, wherein the candidates evaluated by the evaluation means are displayed with ranking.

6. (Original) An apparatus according to claim 1, wherein the calculation means calculates three-dimensional structure for each candidate.

7. (Original) An apparatus according to claim 6, wherein the calculation means provides the three-dimensional structure by molecular dynamic calculation.

8. (Original) An apparatus according to claim 6, wherein the apparatus further comprises a displaying means for displaying the three dimensional structure.

9. (Original) An apparatus according to claim 1, wherein the apparatus further comprises a second data storing means for storing the fourth data.

10. (Original) An apparatus according to claim 1, wherein the first data enters the first input means, the second data enters the second input means and the fourth data is calculated by the calculation means, and wherein the apparatus estimates the structure of ion by making comparisons between the first data and the third data stored in a database, and between the second and fourth data.

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11. (Currently Amended) An apparatus according to claim 10, wherein the apparatus is able to execute analysis for protein and peptide having amino acid as well as protein, peptide and sugar chain having modified amino acid.

12. (Original) An apparatus according to claim 1, wherein the apparatus is able to distinguish leucine from isoleucine which have amino acids of the same mass.

13. (Original) An apparatus according to claim 1, wherein the apparatus further comprises one of an ion trap unit, a triple quad time-of-flight instrument and a tandem mass spectrometry instrument.

14. (Original) An apparatus for analyzing mass spectrometric data comprising:

a first input means for entering first data measured by mass spectrometry for an ion to be analyzed;

a second input means for entering second data measured by mass spectrometry for first to Nth dissociated ions of the ion;

a data storing means for storing third data of mass spectrometry for a plurality of candidates for the structure of ion; and

an evaluation means for evaluating the candidates,

wherein the evaluation means comprises:

a first selection means for selecting a first candidate for the structure of ion by making a comparison between the first data and the third data stored in the data storing means; and

Appl. No. 10/643,545
Amdt. Dated Feb. 17, 2005
Reply to Office Action of September 22, 2004

PATENT
Atty. Dkt. No. 83394.0012
Customer No. 26021

a second selection means which provides a calculation value of mass spectrometry for a Mth candidate, where M is less than or equal to N, and makes a comparison between a measured value of mass spectrometry for a Mth dissociated ion entered through the second input means and the calculation value, repeating from M equal to 1 to M equal to L, where L is equal to or greater than 2 and less than or equal to N, so that a (M+1)th candidate for the structure of ion can be selected.

15. (Original) An apparatus for analyzing mass spectrometric data comprising:

an input means for entering one of first data measured by mass spectrometry for an ion to be analyzed and second data measured by mass spectrometry for a dissociated ion of the ion;

first public data of mass spectrometry for candidates for the structure of ion accessible by internet; and

second public data of mass spectrometry for the structure of dissociated ion for each candidate accessible by internet,

wherein the apparatus evaluates the candidates by making one of comparisons between the first data and first public data and between the second data and second public data, so that the structure of ion can be identified.

16. (Original) A method for analyzing mass spectrometric data, the method comprising the steps of:

measuring first data of mass spectrometry for an ion to be analyzed;

measuring second data of mass spectrometry for a dissociated ion of the ion;

storing third data of mass spectrometry for a plurality of candidates for the structure of ion;

Appl. No. 10/643,545
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Reply to Office Action of September 22, 2004

PATENT
Atty. Dkt. No. 83394.0012
Customer No. 26021

calculating fourth data of mass spectrometry for dissociated ions to be used in analyzing the plurality of candidates for the structure of ion; and

estimating the structure of ion by making comparisons between the first and third data, and between the second and fourth data.

17. (Original) A method according to claim 16, wherein the method is able to distinguish leucine from isoleucine which have amino acids of the same mass.

18. (Original) A system for analyzing compound structure comprising:

a means for conducting mass spectrometry for an ion to be analyzed and a dissociated ion of the ion; and

an apparatus for analyzing mass spectrometric data,

wherein the apparatus comprises:

a first input means for entering first data measured by mass spectrometry for an ion to be analyzed;

a second input means for entering second data measured by mass spectrometry for a dissociated ion of the ion;

a data storing means for storing third data of mass spectrometry for a plurality of candidates for the structure of ion;

a calculation means for producing fourth data of mass spectrometry for dissociated ions to be used in analyzing the plurality of candidates for the structure of ion; and

an evaluation means for evaluating the candidates by making comparisons between the first and third data, and between the second and fourth data, so that the structure of ion can be identified.

Appl. No. 10/643,545
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Customer No. 26021

19. (Original) A system according to claim 18, wherein the system is able to distinguish leucine from isoleucine which have amino acids of the same mass.

20. (Original) A computer program for a computer used for a system for analyzing compound structure, wherein the computer program executes the steps of:

measuring first data of mass spectrometry for an ion to be analyzed;

measuring second data of mass spectrometry for a dissociated ion of the ion;

storing third data of mass spectrometry for a plurality of candidates for the structure of ion;

calculating fourth data of mass spectrometry for dissociated ions to be used in analyzing the plurality of candidates; and

estimating the structure of the ion by making comparisons between the first and third data, and between the second and fourth data.